

Planar and Surface Graphical Models which are EASY

Vladimir Chernyak^(1,2) and Michael Chertkov¹

¹ Center for Nonlinear Studies & Theory Division, LANL
² Chemistry Department, Wayne State, Detroit

"Physics of Algorithms" Workshop Santa Fe, September 1, 2009



Outline

- Introduction
 - Graphical Models
 - Easy and Difficult
 - Dimer and Ising Models on Planar Graphs
- Planar is not necessarily easy ... but
 - Holographic Algorithms & Gauge Transformations
 - Edge-Binary models of degree ≤ 3
 - Edge-Binary Wick Models (of arbitrary degree)
- 3 Surface-Easy
 - Kasteleyn Conjecture for Dimer Model on Surface Graphs
 - Edge-Binary Graph-Model which are Surface-Easy
- 4 Conclusions & Path forward
 - Main "take home" message
 - Where do we go from here?

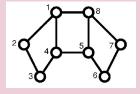


Binary Graphical Models

Forney style - variables on the edges

$$\mathcal{P}(\vec{\sigma}) = Z^{-1} \prod_{a} f_{a}(\vec{\sigma}_{a})$$

$$Z = \sum_{\sigma} \prod_{a} f_{a}(\vec{\sigma}_{a})$$
partition function



$$f_a \ge 0$$

$$\sigma_{ab} = \sigma_{ba} = \pm 1$$

$$\vec{\sigma}_1 = (\sigma_{12}, \sigma_{14}, \sigma_{18})$$

$$\vec{\sigma}_2 = (\sigma_{12}, \sigma_{23})$$

- Most Probable Configuration = Maximum Likelihood = Ground State: $\arg \max \mathcal{P}(\vec{\sigma})$
- Marginal Probability: e.g. $\mathcal{P}(\sigma_{ab}) \equiv \sum_{\vec{\sigma} \setminus \sigma_{ab}} \mathcal{P}(\vec{\sigma})$
- Partition Function: Z Our main object of interest



Easy & Difficult Boolean Problems

EASY

- Any graphical problems on a tree (Bethe-Peierls, Dynamical Programming, BP, TAP and other names)
- Ground State of a Rand. Field Ferrom. Ising model on any graph
- Partition function of planar Ising & Dimer models
- Finding if 2-SAT is satisfiable
- Decoding over Binary Erasure Channel = XOR-SAT
- Some network flow problems (max-flow, min-cut, shortest path, etc)
- Minimal Perfect Matching Problem
- Some special cases of Integer Programming (TUM)

Typical graphical problem, with loops and factor functions of a general position, is DIFFICULT

Glassy Ising & Dimer Models on a Planar Graph

Partition Function of $J_{ij} \geqslant 0$ Ising Model, $\sigma_i = \pm 1$

$$Z = \sum_{\vec{\sigma}} \exp\left(\frac{\sum_{(i,j)\in\Gamma} J_{ij}\sigma_i\sigma_j}{T}\right)$$



Partition Function of Dimer Model, $\pi_{ij} = 0, 1$

$$Z = \sum_{ec{\pi}} \prod_{(i,j) \in \Gamma} (z_{ij})^{\pi_{ij}} \prod_{i \in \Gamma} \delta \left(\sum_{j \in i} \pi_{ij}, 1
ight)$$

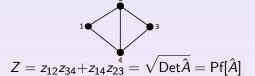


Ising & Dimer Classics

- L. Onsager, Crystal Statistics, Phys.Rev. 65, 117 (1944)
- M. Kac, J.C. Ward, A combinatorial solution of the Two-dimensional Ising Model, Phys. Rev. 88, 1332 (1952)
- C.A. Hurst and H.S. Green, New Solution of the Ising Problem for a Rectangular Lattice, J. of Chem. Phys. 33, 1059 (1960)
- M.E. Fisher, Statistical Mechanics on a Plane Lattice, Phys.Rev 124, 1664 (1961)
- P.W. Kasteleyn, The statistics of dimers on a lattice, Physics 27, 1209 (1961)
- P.W. Kasteleyn, Dimer Statistics and Phase Transitions, J. Math. Phys. 4, 287 (1963)
- M.E. Fisher, On the dimer solution of planar Ising models, J. Math. Phys. 7, 1776 (1966)
- F. Barahona, On the computational complexity of Ising spin glass models,
 J.Phys. A 15, 3241 (1982)



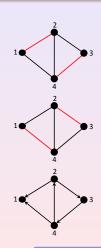
Pfaffian solution of the Matching problem



$$\hat{A} = \begin{pmatrix} 0 & -z_{12} & 0 & -z_{14} \\ +z_{12} & 0 & +z_{23} & -z_{24} \\ 0 & -z_{23} & 0 & +z_{34} \\ +z_{14} & +z_{24} & -z_{34} & 0 \end{pmatrix}$$

Odd-face [Kasteleyn] rule (for signs)

Direct edges of the graph such that for every internal face the number of edges oriented clockwise is odd



► Fermion/Grassman Representation



Planar Spin Glass and Dimer Matching Problems

The Pfaffian formula with the "odd-face" orientation rule extends to any planar graph thus proving constructively that

- Counting weighted number of dimer matchings on a planar graph is easy
- Calculating partition function of the spin glass Ising model on a planar graph is easy

Planar is generally difficult

[Barahona '82]

- Planar spin-glass problem with magnetic field is difficult
- Dimer-monomer matching is difficult even in the planar case



Outline

- Introduction
 - Graphical Models
 - Easy and Difficult
 - Dimer and Ising Models on Planar Graphs
- Planar is not necessarily easy ... but
 - Holographic Algorithms & Gauge Transformations
 - Edge-Binary models of degree ≤ 3
 - Edge-Binary Wick Models (of arbitrary degree)
- 3 Surface-Easy
 - Kasteleyn Conjecture for Dimer Model on Surface Graphs
 - Edge-Binary Graph-Model which are Surface-Easy
- 4 Conclusions & Path forward
 - Main "take home" message
 - Where do we go from here?



Are there other graphical models which are easy?

Holographic Algorithms

[Valiant '02-'08]

- reduction to dimers via
- "classical" one-to-one gadgets

(e.g. Ising model to dimer model)

- "holographic" gadgets (e.g. Ice model to Dimer model)
- resulted in discovery of variety of new easy planar models

Gauge Transformations

[Chertkov, Chernyak '06-'09]

- Equivalent to the holographic gadgets Gauge Transformations (different gauges = different transformations)
- Belief Propagation (BP) Loop Calculus/Series
 is one special choice of the gauge freedom

Are there other graphical models which are easy?

Holographic Algorithms

[Valiant '02-'08]

- reduction to dimers via
- "classical" one-to-one gadgets
 (e.g. Ising model to dimer model)
- "holographic" gadgets (e.g. lce model to Dimer model)
- resulted in discovery of variety of new easy planar models

Gauge Transformations

[Chertkov, Chernyak '06-'09]

- Equivalent to the holographic gadgets Gauge Transformations (different gauges = different transformations)
- Belief Propagation (BP) Loop Calculus/Series
 is one special choice of the gauge freedom

Are there other graphical models which are easy?

Holographic Algorithms

[Valiant '02-'08]

- reduction to dimers via
- "classical" one-to-one gadgets
 (e.g. Ising model to dimer model)
- "holographic" gadgets (e.g. Ice model to Dimer model)
- resulted in discovery of variety of new easy planar models

Gauge Transformations

[Chertkov, Chernyak '06-'09]

- Equivalent to the holographic gadgets Gauge Transformations (different gauges = different transformations)
- Belief Propagation (BP)
 Loop Calculus/Series
 is one special choice of the gauge freedom

BP+ for Planar [degree ≤ 3]

Loop Series (general) [MC,Chernyak '06]

$$Z = Z_0 \cdot z, \ z \equiv 1 + \sum_C r_C$$



Summing 2-regular (closed curve) partition is easy!! [MC, Chernyak, Teodorescu '08]

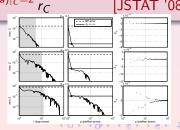
$$Z_s = Z_0 \cdot z_s, \quad z_s = 1 + \sum_{C \in \mathcal{G}}^{\forall a \in C, |\delta(a)|_C = 2} r_C$$

[JSTAT '08]

Efficient Approximate Scheme [Gomez, MC, Kappen '09]

http://arXiv.org/abs/0901.0786

UAI, 2009 + submitted to JML



Easy Models of degree ≤ 3 [MC,Chernyak,Teodorescu '08]

Generic planar problem is difficult

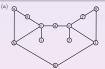
A planar problem is easy if

the factor functions satisfy

$$\forall \ a \in \mathcal{G} : \sum_{\vec{\sigma}_{a}} f_{a}(\vec{\sigma}_{a}) \times \prod_{b}^{(a,b) \in \mathcal{E}} \exp(\eta_{ab}\sigma_{ab})$$
$$\times (\sigma_{ab} - \tanh(\eta_{ab} + \eta_{ba})) = 0$$

where η are messages from a BP solution for the model

• i.e. when all (!!) "three-colorings" are zero after a BP-transformation [BP gauge= all (!!) "one-colorings" are zero]







"three-colorings" are shown in red

Easy Models of degree ≤ 3 (II)

To describe the family of easy edge-binary models of degree not larger than three (partition function is reducible to Pfaffian of a $|\mathcal{G}_1| \times |\mathcal{G}_1|$ -dimensional skew-symmetric matrix) one needs to:

Item #1: Generate an arbitrary factor-function set which satisfies: $\forall a: W^{(a)}(\vec{\sigma}_a) = 0$ if $\sum_{b \geq a} \sigma_{ab} \neq 0 \pmod{2}$



Item #2: Apply an arbitrary skew-orthogonal Gauge-transformation:

$$\begin{split} & W^{(a)}(\pi_a) \to f_a(\pi_a) = \sum_{\pi'_a} \left(\prod_{b \sim a} G_{ab}(\pi_{ab}, \pi'_{ab}) \right) W^{(a)}(\pi'_a) \\ & \forall \{a, b\} \in \mathcal{G}_1 : \sum_{\pi} G_{ab}(\pi, \pi') G_{ba}(\pi, \pi'') = \delta(\pi', \pi'') \\ & Z = \sum_{\pi} \prod_{a \in \mathcal{G}_0} f_a(\pi_a) = \sum_{\pi} \prod_{a \in \mathcal{G}_0} \left(\sum_{\pi'} \left(\prod_{b \sim a} G_{ab}(\pi_{ab}, \pi'_{ab}) \right) W^{(a)}(\pi_a) \right) \end{split}$$

Next Step:

Generalize construction (Item #1) to degree > 3 [Item #2 is already generic]



Edge Binary Wick (EBW) Models

[Chernyak, MC '09]

$$Z_{EBW}(W) = \sum_{\gamma = \{\gamma_{ab}\} \in \mathcal{Z}_1(\mathcal{G}; \mathbb{Z}_2)} \prod_{b \in \mathcal{G}_0}^{\sum_{a \sim b} \gamma_{ab} \neq 0} W_{\{a_1, \cdots, a_{2k}\} \equiv \{a \mid a \sim b; \gamma_{ab} = 1\}}^{(b)}$$



- All odd weights are zero
- Even (d > 2) weights are expressed

number of crossings (mod 2)

$$\sum_{p,p'\in\xi}^{p$$

Examples of 6-colorings and extensions of a EBW-model 6 vertex









 $W_{16}W_{25}W_{34}$ [zero crossing]

 $-W_{12}W_{35}W_{46}$ [one crossing]

 $W_{13}W_{25}W_{46}$ [two crossings] $-W_{14}W_{25}W_{36}$ [three crossings]

◆ロ → ◆ 個 → ◆ 量 → ◆ 量 | ■ り へ ○

Edge Binary Wick Models (II)

Known Easy Planar Graphical Models & EBW

- \exists a gauge transformation reducing any easy planar model to a EBW
 - Dimer Model
 - Ising Model
 - Ice Model
 - Possibly all models discussed in the "holographic" papers

Any EBW model on a planar graph is EASY

- Equivalent to Gaussian Grassman Models on the same graph
- ullet Partition function is Pfaffian of a $|\mathcal{G}_1| imes |\mathcal{G}_1|$ matrix



Related Grassmann/Fermion Models

Vertex Gaussian Grassmann Graphical (VG³) Models

$$\begin{split} Z_{\text{VG}^{3}}(\varsigma, \sigma; \mathbf{W}) &= \frac{\int \exp\left(\frac{1}{2} \sum\limits_{(b \to a \to c) \in \mathcal{G}_{1}} \varphi_{ab} \varsigma_{bc}^{(a)} W_{bc}^{(a)} \varphi_{ac}\right) \exp\left(\frac{1}{2} \sum_{(a,b) \in \mathcal{G}_{1}} \varphi_{ab} \sigma_{ab} \varphi_{ba}\right) \prod\limits_{(a,b)} d\varphi_{ab}}{\int \exp\left(\frac{1}{2} \sum_{(a,b) \in \mathcal{G}_{1}} \varphi_{ab} \sigma_{ab} \varphi_{ba}\right) \prod\limits_{(a,b)} d\varphi_{ab}} \\ &= \frac{\Pr(H(\varsigma, \sigma; \mathbf{W}))}{\Pr(H(\varsigma, \sigma; \mathbf{O}))}, \qquad H_{ij} = \left\{ \begin{array}{cc} \varsigma_{bc}^{(a)} W_{bc}^{(a)}, & i = (a,b) \& j = (a,c), \text{ where } b \neq c \sim a, \\ \sigma_{ab}, & i = (a,b), \& j = (b,a). \end{array} \right. \end{split}$$

Grassmann (anti-commuting) variables: $\forall (a,b), (c,d) \in \mathcal{G}_1 \quad \varphi_{ab}\varphi_{cd} = -\varphi_{cd}\varphi_{ab}$ Berezin (formal) integration rules: $\forall (a,b) \in \mathcal{G}_1 : \int d\varphi_{ab} = 0, \quad \int \varphi_{ab} d\varphi_{ab} = 1$

Main Theorem of [Chernyak, MC '09/planar]

- $\exists \sigma, \varsigma = \pm 1$: s.t. $Z_{VG^3}(\varsigma, \sigma; \mathbf{W}) = Z_{EBW}(\mathbf{W})$
- The special configuration of σ, ς corresponds to Kastelyan (spinor) orientation on the extended planar graph

Outline

- Introduction
 - Graphical Models
 - Easy and Difficult
 - Dimer and Ising Models on Planar Graphs
- Planar is not necessarily easy ... but
 - Holographic Algorithms & Gauge Transformations
 - Edge-Binary models of degree ≤ 3
 - Edge-Binary Wick Models (of arbitrary degree)
- 3 Surface-Easy
 - Kasteleyn Conjecture for Dimer Model on Surface Graphs
 - Edge-Binary Graph-Model which are Surface-Easy
- 4 Conclusions & Path forward
 - Main "take home" message
 - Where do we go from here?

Dimer Model on Surface Graphs (I)

Partition function of dimer model on a surface graph of genus g is expressed in terms of a (± 1) -weighted sum over 2^{2g} determinants = surface-easy

- Kasteleyn '63;'67 non-constructive (??) conjecture
- Gallucio, Loebl '99 first [combinatorial] proof
- Cimasoni, Reshetikhin '07 topological proof and relation to gauge fermion models



genus g = 0



genus g=1



genus g=2

Dimer Model on Surface Graphs (II)

Partition Function of Dimer Model, $\pi_{ij}=0,1$, on a surface graph ${\cal G}$

$$Z(\mathcal{G}; \mathbf{z}) = \sum_{\vec{\pi}}^{\text{dimers}} \prod_{(i,j) \in \Gamma} (z_{ij})^{\pi_{ij}}$$

Theorem: (formulation of Cimasoni, Reshetikhin)

$$Z(\mathcal{G}; \mathbf{z}) = \frac{1}{2^g} \sum_{[\mathbf{s}]} \underbrace{\operatorname{Arf}(q_{\pi_0}^{\mathbf{s}}) \varepsilon^{\mathbf{s}}(\pi_0)}_{\mathsf{Pf}(A^{\mathbf{s}}(z))}$$

 $=\pm 1; \ \pi_0-independent;$ depends only on [s]

- π_0 is a reference dimer configuration
- s is a Kasteleyn orientation; [s] equivalence classes of the Kasteleyn orientations,
 2^{2g} of them
- $\varepsilon^{\mathbf{s}}(\pi)=\pm 1$ defines total signature of the dimer configuration π wrt the Kasteleyn orientation \mathbf{s}
- $q_{\pi_0}^{\mathbf{s}}(\alpha)$ is a well-defined quadratic form associated with \mathbf{s} , π_0 and α is a closed curve on \mathcal{G} ; $\mathrm{Arf}(q_{\pi_0}^{\mathbf{s}})$ is the Arf-invariant of the quadratic form.

Dimer Model on Surface Graphs (III)

[Cimasoni, Reshetikhin]

$$Z(\mathcal{G}; \mathbf{z}) = rac{1}{2^{\varepsilon}} \sum_{[\mathbf{s}]} \mathsf{Arf}(q^{\mathbf{s}}_{m{\pi}_0}) arepsilon^{\mathbf{s}}(m{\pi}_0) \mathsf{Pf}(A^{\mathbf{s}}(z))$$

- the sum over determinants can be transformed into the sum over partition functions of Kasteleyn-fermion models
- Kasteleyn orientation is a discrete version of spin(or) structures [from topological field theories]
- Powerful derivation techniques from topology [homology and immersion theories]

Generic graphical model on a surface graph is SURFACE-DIFFICULT

Our next task is:

To classify graphical models which are SURFACE-EASY

Edge-Binary-Wick (EBW) Models and Vertex Gaussian Grassman Graphical (VG³) models on Surface Graphs

Main Theorem of [Chernyak, MC '09/surface]

$$Z_{EBW}(\mathbf{W})Z_{EBW}(\mathbf{1}) = \sum_{[\mathbf{s}]} Z_{VG^3}([\mathbf{s}];\mathbf{1})Z_{VG^3}([\mathbf{s}];\mathbf{W})$$
 where

- $\mathbf{s} = (\boldsymbol{\sigma}; \boldsymbol{\varsigma})$ corresponds to a Kastelyan/spinor orientation defined on extended graph
- [s] are equivalence classes (2^{2g} of them) of the Kastelyan/spinor s
 orientations







EBW and VG³ models on Surface Graphs (II)

$$Z_{EBW}(\mathbf{W})Z_{EBW}(\mathbf{1}) = \sum_{[\mathbf{s}]} Z_{VG^3}([\mathbf{s}];\mathbf{1})Z_{VG^3}([\mathbf{s}];\mathbf{W})$$

The multi-step proof of the main surface theorem includes

- Extended/fat graph construction and partitioning ξ of the even generalized loop γ configurations into closed curves [Wick structure]
- Analysis and relation between invariant objects (quadratic forms) for the generalized loops, [\gamma], and spinors, [s], defined on fat graphs and respective Riemann surfaces.
- Term by term comparison of the relation between the partial $\tilde{Z}_{EBW}([\gamma]; \mathbf{W})$ and $\tilde{Z}_{VG^3}([\gamma], [\mathbf{s}]; \mathbf{W})$, where $Z_{EBW}(\mathbf{W}) = \sum_{[\gamma]} \tilde{Z}_{EBW}([\gamma]; \mathbf{W})$ and $Z_{VG^3}([\mathbf{s}]; \mathbf{W}) = \sum_{[\gamma]} \tilde{Z}_{VG^3}([\gamma], [\mathbf{s}]; \mathbf{W})$. This results in the system of 2^{2g} linear equations for 2^{2g} unknowns $\tilde{Z}_{EBW}([\gamma]; \mathbf{W})$.
- Solving the linear equations we recover the main statement of the theorem.
- $2^g Z_{VG^3}([s]; 1) = Arf(q([s]))Z_{EBW}(1)$, where $q(s)(\gamma) = q([s])([\gamma])$ is a well-defined quadratic form.

Q:

Describe the family of surface-easy edge-binary models on an arbitrary surface graph \mathcal{G} (partition function is reducible to a sum of 2^{2g} Pfaffians)

A: [constructive]

- Generate an arbitrary Vertex Gaussian Grassmann binary-Gauge (VG³) Model on the graph
- Fix the binary-gauge according to the Kasteleyn (spinor) rule on the extended graph
- Construct respective Edge-Binary Wick model on the original graph
- Apply an arbitrary skew-orthogonal (holographic) gauge/transformation

The partition function of the resulting model is the sum of $2^{2g} \pm$ -weighted Pfaffians. [All terms in the sum are explicitly known.]

Future work

- Use the described hierarchy of easy planar models as a basis for efficient <u>variational approximation</u> of generic (difficult) planar problems. (The approach may also be useful for building efficient variational matrix-product state wave functions for <u>quantum models</u>. Dynamical Bayesian Networks: 1+1, tree+1,)
- Study Wick Gaussian models on non-planar but
 <u>Pfaffian orientable</u> or k-Pfaffian orientable graphs (where any dimer model on surface graph of genus g is 2^{2g}-Pfaffian orientable).
- Almost Planar = Geographical Graphical Models, Renormalization Group, Generalized BP
- Analogs of all of the above for Surface-Difficult Problems

Example (1): Statistical Physics

Ising model

$$\sigma_i = \pm 1$$

$$\mathcal{P}(\vec{\sigma}) = \mathbf{Z}^{-1} \exp\left(\sum_{(i,j)} J_{ij} \sigma_i \sigma_j\right)$$

 J_{ij} defines the graph (lattice)

Graphical Representation

Variables are usually associated with vertexes ... but transformation to the Forney graph (variables on the edges) is straightforward

- ullet Ferromagnetic $(J_{ij} < 0)$, Anti-ferromagnetic $(J_{ij} > 0)$ and Frustrated/Glassy
- Magnetization (order parameter) and Ground State
- Thermodynamic Limit, $N \to \infty$
- Phase Transitions

Example (2): Information Theory, Machine Learning, etc

Probabilistic Reconstruction (Statistical Inference)

 $ec{\sigma}_{\mathsf{orig}}$

 \Rightarrow

 $\vec{\sigma}$

original data $ec{\sigma}_{ t orig} \in \mathcal{C}$

codeword

noisy channel $\mathcal{P}(\vec{x}|\vec{\sigma})$

corrupted data:

log-likelihood magnetic field statistical inference

possible preimage $\vec{\sigma} \in \mathcal{C}$

Maximum Likelihood

Marginalization

$$\mathsf{ML}(\vec{x}) = \arg\max_{\vec{\sigma}} \mathcal{P}(\vec{x}|\vec{\sigma})$$

$$\sigma_i^*(\vec{x}) = \arg\max_{\sigma_i} \sum_{\vec{\sigma} \setminus \sigma_i} \mathcal{P}(\vec{x} | \vec{\sigma})$$

Counting (Partition Function): $Z(\vec{x}) = \sum_{\vec{\sigma}} P(\vec{x}|\vec{\sigma})$

Example (2): Information Theory, Machine Learning, etc.

Probabilistic Reconstruction (Statistical Inference)

 $\mathcal{P}(\vec{x}|\vec{\sigma})$

 \vec{x}

noisy channel

corrupted

data: log-likelihood

magnetic field

statistical inference

possible preimage $\vec{\sigma} \in \mathcal{C}$

$$ML(\vec{x}) = \arg \max_{\vec{\sigma}} \mathcal{P}(\vec{x}|\vec{\sigma})$$

$$\sigma_i^*(ec{x}) = rg \max_{\sigma_i} \sum_{ec{\sigma} \setminus \sigma_i} \mathcal{P}(ec{x} | ec{\sigma})$$

Example (2): Information Theory, Machine Learning, etc

magnetic field

Maximum Likelihood

${\sf Marginalization}$

$$\mathsf{ML}(ec{x}) = \arg\max_{ec{\sigma}} \mathcal{P}(ec{x}|ec{\sigma})$$
 $\sigma_i^*(ec{x}) = \arg\max_{\sigma_i} \sum_{ec{\sigma} \setminus \sigma_i} \mathcal{P}(ec{x}|ec{\sigma})$

Counting (Partition Function): $Z(\vec{x}) = \sum_{\vec{\sigma}} P(\vec{x}|\vec{\sigma})$

Example (2): Information Theory, Machine Learning, etc

Probabilistic Reconstruction (Statistical Inference)

 $orig \Rightarrow$

 \vec{x}

 \Rightarrow

 $\vec{\sigma}$

original

no

noisy channel $\mathcal{P}(\vec{x}|\vec{\sigma})$

 $\mathcal{P}(\vec{x}|\vec{\sigma})$

corrupted

data:

log-likelihood magnetic field statistical inference

possible preimage $\vec{\sigma} \in \mathcal{C}$

 σ

Maximum Likelihood Iground state

Marginalization

$$\mathsf{ML}(\vec{x}) = \arg\max_{\vec{\sigma}} \mathcal{P}(\vec{x}|\vec{\sigma})$$

$$\sigma_i^*(\vec{x}) = \arg\max_{\sigma_i} \sum_{\vec{\sigma} \setminus \sigma_i} \mathcal{P}(\vec{x}|\vec{\sigma})$$

Counting (Partition Function): $Z(\vec{x}) = \sum_{\vec{\sigma}} P(\vec{x}|\vec{\sigma})$

Grassmann (fermion, nilpotent) Calculus for Pfaffians

Grassman (nilpotent) Variables on Vertexes

$$\forall (a,b) \in \mathcal{G}_e: \quad \theta_a \theta_b + \theta_b \theta_a = 0 \quad \int d\theta = 0, \quad \int \theta d\theta = 1$$

Pfaffian as a Gaussian Berezin Integral over the Fermions

$$\int \exp\left(-\frac{1}{2}\vec{\theta}^t\hat{A}\vec{\theta}\right)d\vec{\theta} = \mathsf{Pf}(\hat{A}) = \sqrt{\mathsf{det}(\hat{A})}$$

◆ Pfaffian Formula

Local Gauge, G, Transformations



$$Z = \sum_{\vec{\sigma}} \prod_{a} f_{a}(\vec{\sigma}_{a}), \ \vec{\sigma}_{a} = (\sigma_{ab}, \sigma_{ac}, \cdots)$$

$$\sigma_{ab} = \sigma_{ba} = \pm 1$$

$$f_{a}(\vec{\sigma}_{a} = (\sigma_{ab}, \cdots)) \rightarrow \sum_{\sigma'_{ab}} G_{ab}(\sigma_{ab}, \sigma'_{ab}) f_{a}(\sigma'_{ab}, \cdots)$$

$$\sum_{\sigma_{ab}} G_{ab}(\sigma_{ab}, \sigma') G_{ba}(\sigma_{ab}, \sigma'') = \delta(\sigma', \sigma'')$$

The partition function is invariant under any G-gauge!

$$Z = \sum_{\vec{\sigma}} \prod_{a} f_a(\vec{\sigma}_a) = \sum_{\vec{\sigma}} \prod_{a} \left(\sum_{\vec{\sigma}'_a} f_a(\vec{\sigma}'_a) \prod_{b \in a} G_{ab}(\sigma_{ab}, \sigma'_{ab}) \right)$$

Belief Propagation as a Gauge Fixing Chertkov, Chernyak '06

$$Z = \sum_{\vec{\sigma}} \prod_{a} f_a(\vec{\sigma}_a) = \sum_{\sigma} \prod_{a} \left(\sum_{\vec{\sigma}'_a} f_a(\vec{\sigma}'_a) \prod_{b \in a} G_{ab}(\sigma_{ab}, \sigma'_{ab}) \right)$$

$$Z = \underbrace{Z_0(G)}_{\text{ground state}} + \underbrace{\sum_{\text{all possible colorings of the graph}} Z_c(G)}_{\vec{\sigma} = +\vec{1}} + \underbrace{\sum_{\vec{\sigma} \neq +\vec{1}, \text{excited states}} Z_c(G)}_{\vec{\sigma} \neq +\vec{1}, \text{excited states}}$$

Belief Propagation Gauge

$\forall a \& \forall b \in a$:

$$\sum_{\vec{\sigma'}_a} f_a(\vec{\sigma'}) G_{ab}^{(bp)}(\sigma_{ab} = -1, \sigma'_{ab}) \prod_{c \in a}^{c \neq b} G_{ac}^{(bp)}(+1, \sigma'_{ac}) = 0$$

No loose BLUE=colored edges at any vertex of the graph!

Belief Propagation as a Gauge Fixing (II)

$\forall a \& \forall b \in a$:

$$\left\{ \begin{array}{l} \sum\limits_{\sigma',a} f_{a}(\vec{\sigma}') G_{ab}^{(bp)}(-1,\sigma'_{ab}) \prod\limits_{c \in a}^{c \neq b} G_{ac}^{(bp)}(+1,\sigma'_{ac}) = 0 \\ \sum\limits_{\sigma,ab} G_{ab}(\sigma_{ab},\sigma') G_{ba}(\sigma_{ab},\sigma'') = \delta(\sigma',\sigma'') \end{array} \right. \Rightarrow \left\{ \begin{array}{l} \sum\limits_{sum-product} \sigma_{ab}^{(bp)}(+1,\sigma'_{ab}) = \rho_{a}^{-1} \sum\limits_{\sigma',a} f_{a}(\vec{\sigma}') \prod\limits_{c \in a} G_{ac}^{(bp)}(+1,\sigma'_{ac}) \\ \rho_{a} = \sum\limits_{\sigma',a} f_{a}(\vec{\sigma}') \prod\limits_{c \in a} G_{ac}^{(bp)}(+1,\sigma'_{ac}) \end{array} \right.$$

Belief Propagation in terms of Messages

$$G_{ab}^{(bp)}(\underbrace{+1},\sigma) = \frac{\exp\left(\sigma\eta_{ab}\right)}{2\sqrt{\cosh(\eta_{ab}+\eta_{ba})}}, \quad G_{ab}^{(bp)}(-1,\sigma) = \sigma\frac{\exp\left(-\sigma\eta_{ba}\right)}{2\sqrt{\cosh(\eta_{ab}+\eta_{ba})}} \Longrightarrow$$

$$\sum_{\vec{\sigma}_{a} \setminus \sigma_{ab}} f_{a}(\vec{\sigma}_{a}) \exp \left(\sum_{c \in a} \sigma_{ac} \eta_{ac} \right) \left(\sigma_{ab} - \tanh \left(\eta_{ab} + \eta_{ba} \right) \right) = 0$$

$$b_a(\vec{\sigma}_a) = \frac{f_a(\vec{\sigma}_a) \exp\left(\sum_{b \in a} \sigma_{ab} \eta_{ab}\right)}{\sum_{\vec{\sigma}_a} f_a(\vec{\sigma}_a) \exp\left(\sum_{b \in a} \sigma_{ab} \eta_{ab}\right)}, \quad b_{ab}(\sigma) = \frac{\exp(\sigma(\eta_{ab} + \eta_{ba}))}{\sum_{\sigma} \exp(\sigma(\eta_{ab} + \eta_{ba}))}$$

$$\rightarrow \text{Holographic Gadgets \& Gauges}$$

Exact (!!) expression in terms of BP

$$Z = \sum_{\vec{\sigma}_{\sigma}} \prod_{a} f_{a}(\vec{\sigma}_{a}) = Z_{0} \left(1 + \sum_{C} r(C) \right)$$
$$r(C) = \frac{\prod_{a \in C} \mu_{a}}{\prod_{a} (1 - m_{ab}^{2})} = \prod_{c \in C} \tilde{\mu}_{a}$$

 $C \in Generalized Loops = Loops without loose ends$

$$\begin{split} m_{ab} &= \sum_{\vec{\sigma}_a} b_a^{(bp)} (\vec{\sigma}_a) \sigma_{ab} \\ \mu_a &= \sum_{\vec{\sigma}_a} b_a^{(bp)} (\vec{\sigma}_a) \prod_{b \in a, C} (\sigma_{ab} - m_{ab}) \end{split}$$



- The Loop Series is finite
- All terms in the series are calculated within BP
- BP is exact on a tree
- BP is a Gauge fixing condition.
 Other choices of Gauges would lead to different representation.

▶ Holographic Gadgets & Gauges

Ice Model [vertexes of max degree 3]

#PL-3-NAE-ICE

[Valiant '02]

- Input: A planar graph G = (V;E) of maximum degree 3.
- Output: The number of orientations (arrows) such that no node has all the edges directed towards it or away from it.

From arrows to binary variables

- Edge {a, b} is broken in two by insertion of a − b vertex
- Introduce binary variables s.t. if $a \rightarrow b \Rightarrow \pi_{a,a-b} = 0, \pi_{b,a-b} = 1$ $b \rightarrow a \Rightarrow \pi_{a,a-b} = 1, \pi_{b,a-b} = 0$

$$Z_{ice} = \sum_{\boldsymbol{\pi}'} \left(\prod_{a \in \mathcal{G}_0} f_a(\tilde{\boldsymbol{\pi}}_a) \right) \left(\prod_{\{a,b\} \in \mathcal{G}_1} g_{a-b}(\pi_{a,a-b}, \pi_{b,a-b}) \right)$$

$$f_{a}(\pi'_{a}) = \begin{cases} 1, & \exists \ b, c \in \delta_{\mathcal{G}}(a), \quad \text{s.t.} \quad \pi_{a,a-b} \neq \pi_{a,a-c} \\ 0, & \text{otherwise} \end{cases}$$

$$g_{a-b}(\pi'_a) = \begin{cases} 1 & \pi_{a,a-b} \neq \pi_{b,a-b} \\ 0, & \text{otherwise} \end{cases}$$

Holographic Gadgets & Gauges



Ice Model [vertexes of max degree 3] II

General Gauge Transformation

$$\begin{split} f_{a}(\boldsymbol{\pi}_{a}) &\rightarrow \tilde{f}_{a}(\boldsymbol{\pi}_{a}) = \sum_{\boldsymbol{\pi}_{a}'} \left(\prod_{b \sim a} G_{ab}(\boldsymbol{\pi}_{ab}, \boldsymbol{\pi}_{ab}') \right) f_{a}(\boldsymbol{\pi}_{a}') \\ \forall \{a, b\} \in \mathcal{G}_{1} : \sum_{\boldsymbol{\pi}} G_{ab}(\boldsymbol{\pi}, \boldsymbol{\pi}') G_{ba}(\boldsymbol{\pi}, \boldsymbol{\pi}'') = \delta(\boldsymbol{\pi}', \boldsymbol{\pi}'') \\ Z &= \sum_{\boldsymbol{\pi}} \prod_{a \in \mathcal{G}_{0}} \tilde{f}_{a}(\boldsymbol{\pi}_{a}) = \sum_{\boldsymbol{\pi}} \prod_{a \in \mathcal{G}_{0}} \left(\sum_{\boldsymbol{\pi}_{a}'} \left(\prod_{b \sim a} G_{ab}(\boldsymbol{\pi}_{ab}, \boldsymbol{\pi}_{ab}') \right) f_{a}(\boldsymbol{\pi}_{a}) \right) \end{split}$$

Gauge Transformation for the Ice model

$$\begin{split} G_{a,a-b}^{(ice)} &= \frac{1}{\sqrt{2}} \left(\begin{array}{cc} 1 & 1 \\ -1 & 1 \end{array} \right) \quad \tilde{g}_{a-b}(\pi_a') = \left\{ \begin{array}{cc} 1, & \pi_{a,a-b} = \pi_{b,a-b} = 0 \\ -1, & \pi_{a,a-b} = \pi_{b,a-b} = 1 \\ 0, & \text{otherwise} \end{array} \right. \\ \tilde{f}_{a}(\pi_{a,a-1}, \pi_{a,a-2}, \pi_{a,a-3}) &= \frac{3}{\sqrt{2}} * \left\{ \begin{array}{cc} 1, & \pi_{a,a-1} = \pi_{a,a-2} = \pi_{a,a-3} = 0 \\ -1/3, & \sum_{i} \pi_{a,a-i} = 2 \\ 0, & \text{otherwise} \end{array} \right. \end{split}$$